

# Graphs with Extremal Randić Index

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## Definitions and notations :

The **Randić index**  $R(G)$  of a graph  $G$  was introduced by the chemist **Milan Randić** in 1975,

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d(u)d(v)}},$$

where  $d(u)$  denotes the degree of a vertex  $u$  in  $G$ .

There are many different kinds of chemical indices. Some of them are distance based indices (Wiener index), some are degree based indices (Randić index).

Different indices have different use in chemistry.

There is a good correlation between **Randić index** and several **physicochemical properties** of alkanes : **boiling points, surface areas, energy levels**, etc.

Recently, finding bounds for the Randić index of a given class of graphs, as well as related problem of finding the graphs with extremal Randić index, attracted the attention of many researchers, and many results have been obtained.

X. Li, I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, *Mathematical Chemistry Monographs No.1*, Kragujevac, 2006, pp.VI+330.

Bollobás and Erdős proved that :

Let  $G$  be a graph of order  $n$ , containing no isolated vertex ( $\delta(G) \geq 1$ ). Then

$$R(G) \geq \sqrt{n-1},$$

with equality if and only if  $G$  is a star.

B. Bollobás and P. Erdős, Graphs of extremal weights,  
Ars Combin. 50(1998), 225–233.

## Question :

Bollobás and Erdős asked for the minimum value of the Randić index for graphs  $G$  with given minimum degree  $\delta(G)$ .

S. Fajtlowicz, Written on the wall, Conjectures of the program galatea gabriella graffiti, University of Houston, 1998.

### Conjecture 1 :

Let  $G = (V, E)$  be a graph of order  $n$  with  $\delta(G) \geq k$ . Then

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2} \frac{1}{n-1}$$

with equality if and only if  $G = K_{k,n-k}^*$ , where  $K_{k,n-k}^*$  is obtained from a complete bipartite graph  $G = K_{k,n-k}$  by joining each pair of vertices in the part with  $k$  vertices by a new edge.

And they proved the case of  $k = 2$ .

C. Delorme, O. Favaron and D. Rautenbach, On the Randić index, *Discrete Math.* 257(2002), 29–38.

C. Delorme et al also proposed that :

Let  $G = (V, E)$  be a triangle-free graph of order  $n$  with  $\delta(G) \geq k$ . Then

$$R(G) \geq \sqrt{k(n - k)},$$

with equality if and only if  $G = K_{k, n-k}$ .

C. Delorme, O. Favaron and D. Rautenbach, On the Randić index, *Discrete Math.* 257(2002), 29–38.

However, H. Liu, M. Lu and F. Tian found a mistake in their proof, and they proved the case of  $k = 2$  which supports the above result.

H. Liu, M. Lu, F. Tian, On the Randić index, J. Math. Chem. 38(3)(2005), 345–354.

Our main results :

**Theorem 1** (1). For  $k = 3$ , the conjecture is true ;  
(2). For  $k \geq 4$ , if  $n \geq \frac{3}{2}k^3$ , the conjecture is true.

Our main method :

the linear programming

**Lemma 1** *Let  $x_1x_2$  be an edge of maximal weight in a graph  $G$ , then  $R(G - x_1x_2) < R(G)$ .*

B. Bollobás and P. Erdős, Graphs of extremal weights,  
*Ars Combin.* 50(1998), 225–233.

By Lemma 1, we have the following Lemma :

**Lemma 2** *Let  $G$  be the graph with minimum Randić index among all simple graphs with order  $n$  and minimum degree  $\delta(G) \geq k \geq 2$ . Then the minimum degree of  $G$  must be  $k$ .*

By Lemma 2, we transform the conjecture to the following form :

### Conjecture 1'

Let  $G = (V, E)$  be a graph of order  $n$  with  $\delta(G) = k$ . Then

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2} \frac{1}{n-1}$$

with equality if and only if  $G = K_{k, n-k}^*$ .

## Some notations :

$x_{i,j}$  : the number of edges joining the vertices of degrees  $i$  and  $j$  ;

$p$  : the number of vertices whose degree is  $n - 1$   
( $0 \leq p \leq k$ ) ;

$n_i$  : the number of vertices with degree  $i$  ;

$R^{(i)}$  : the Randić index of the graph with  $n_{n-1} = i$ .

We need to solve the following problem :

$$\min R(G) = \sum_{\substack{k \leq i \leq n-1 \\ i \leq j \leq n-1}} \frac{x_{i,j}}{\sqrt{ij}}$$

under constraints :

$$x_{j,k} + x_{j,k+1} + \cdots + x_{j,j-1} + 2x_{j,j} + x_{j,j+1} + \cdots + x_{j,n-1} = jn_j \quad (1)$$

$$n_k + n_{k+1} + n_{k+2} + \cdots + n_{n-1} = n \quad (2)$$

$$x_{i,n-1} = n_i n_{n-1} \quad \text{for } i = k, k+1, \cdots, n-2 \quad (3)$$

$$x_{n-1,n-1} = \binom{n_{n-1}}{2}. \quad (4)$$

Since the constraint (3) are quadratic equalities. To avoid the complicity of these quadratic inequalities, we will give  $n_{n-1}$  all possible values and solve the problem :

Case 1 :  $p = k$

Case 2 :  $0 \leq p \leq k - 1$

Case 1 :  $p = k$

We proved that : for  $k \geq 4$ , if  $n \geq \frac{3}{2}k^3$ ,

$$R^{(k)} \geq \binom{k}{2} \frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}},$$

with equality if and only if

$n_k = n - k$ ,  $n_{k+1} = n_{k+2} = \dots = n_{n-2} = 0$ ,  $n_{n-1} = k$ ,  
 $x_{k,n-1} = k(n-k)$ ,  $x_{n-1,n-1} = \binom{k}{2}$  and all other  $x_{i,j}$  and  
 $x_{i,i}$  are equal to 0, i.e.,  $G = K_{k,n-k}^*$ .

Case 2 :  $0 \leq p \leq k - 1$

We proved that : for  $k \geq 4$ , if  $n \geq \frac{3}{2}k^3$ ,

$$R^{(p)} \geq \binom{k}{2} \frac{1}{n-1} + \frac{\sqrt{k}(n-k)}{\sqrt{n-1}}.$$

For the case of  $k = 3$ , we can prove by the same method.

**Thank you !**